

On the resolution of the big bang singularity in isotropic Loop Quantum Cosmology

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Abstract

In contrast to previous work in the field, we construct the Loop Quantum Cosmology (LQC) of the flat isotropic model with a massless scalar field in the absence of higher order curvature corrections to the gravitational part of the Hamiltonian constraint. The matter part of the constraint contains the inverse triad operator which can be quantized with or without the use of a Thiemann- like procedure. With the latter choice, we show that the LQC quantization is identical to that of the standard Wheeler DeWitt theory (WDW) wherein there is no singularity resolution. We argue that the former choice leads to singularity resolution in the sense of a well defined, regular (backward) evolution through and beyond the epoch where the size of the universe vanishes.

Our work along with that of the seminal work of Ashtekar, Pawłowski and Singh (APS) clarifies the role, in singularity resolution, of the three ‘exotic’ structures in this LQC model, namely: curvature corrections, inverse triad definitions and the ‘polymer’ nature of the kinematic representation. We also critically examine certain technical assumptions made by APS in their analysis of WDW semiclassical states and point out some problems stemming from the infrared behaviour of their wave functions.

1 Introduction

In recent years Loop Quantum Gravity (LQG) techniques have been applied to quantize the space of homogeneous and isotropic configurations of the gravitational field [1] and there is growing evidence that in the resulting quantum cosmology (known as Loop Quantum Cosmology or LQC) the big bang singularity is resolved. Here we focus on the LQC of the spatially flat isotropic model coupled to a homogeneous massless scalar field. This model was studied in great detail in the LQC context by Ashtekar, Pawłowski and Singh (APS)[2, 3]. APS consider evolution from a classical epoch back

towards the singularity and show that quantum effects result in a ‘bounce’ which occurs before the universe gets to zero size. This is the sense in which the singularity is resolved in their work.

APS compare the LQC quantization to that of the more conventional Wheeler DeWitt theory. In the framework of the Wheeler DeWitt theory they find that the singularity persists i.e. the universe reaches zero size at which point physical quantities of interest (such as the scalar field density) diverge. It follows that LQC is sufficiently different from conventional quantization schemes, the differences being responsible for singularity resolution. The three key ‘exotic’ features of LQC in the spatially flat model are as follows:

(i) *Discreteness of spatial geometry*: The quantum kinematics is based on an exotic representation (which is the counterpart of the representation used in LQG and) which endows the scale factor operator with a discrete spectrum in contrast to the continuous spectrum obtained in the Wheeler DeWitt case wherein the scale factor operator acts by multiplication, exactly like the position operator in particle quantum mechanics.

(ii) *Curvature corrections*: Analogous to the holonomy operators of LQG, the basic operator of LQC is the exponential of the Ashtekar- Barbero connection [4] (in the flat model under consideration, this connection is just the extrinsic curvature of the spatial slice) and, as a result, the quantum dynamics needs to be re-expressed in terms of these operators. The dynamics is generated by a constraint operator whose gravitational part depends on the extrinsic curvature. Due to the nature of the representation, the extrinsic curvature is not a well defined operator and APS replace this term by appropriately defined approximants which depend on the LQC holonomies. The structure of the holonomy approximants is motivated by definitions of the Hamiltonian constraint operator in full LQG. The approximants agree with the classical general relativistic expression at low curvatures (i.e. in the classical regime) but differ in the high curvature regime in the vicinity of the classical singularity. This leads to a correction to general relativistic dynamics near the singularity which is absent in the Wheeler DeWitt case wherein the extrinsic curvature is a well defined operator.

(iii) *Inverse triad definitions*: The matter part of the constraint depends on the inverse scale factor. In analogy to Thiemann’s procedure in LQG [5] this quantity is first expressed in terms of a Poisson bracket between the ‘holonomy’ and the spatial volume and then promoted to a quantum operator by replacing the Poisson bracket by the quantum commutator. The eigen states of the resultant inverse scale factor operator are identical with those of the scale factor operator. Moreover, the spectrum of the resultant inverse scale factor operator agrees with that of the straightforward inverse

for large eigenvalues of the scale factor but differs when these eigenvalues are small, the eigen value of the former being bounded (and typically vanishing) when the scale factor eigen value vanishes [6, 2, 3].

The primary aim of this work is to clarify the role of the above features in singularity resolution in the isotropic model under consideration. Since we are interested in LQC, all our constructions will be based on (i). APS have already argued persuasively (see [7]) that in this model, the quantum bounce occurs primarily due to (ii) rather than (iii). In this work we use the techniques introduced in Reference [3] to construct an LQC quantization which *does not contain feature (ii)*. We are able to do this both with and without (iii). Our results are as follows.

As in [2, 3] the quantization admits the interpretation of the scalar field as a clock. If one does not introduce feature (iii) i.e. if we use the straightforward scale factor operator inverse defined directly through the spectral decomposition of the scale factor operator with the replacement of each eigen value of the latter by its inverse, we obtain a representation of the physical degrees of freedom which is equivalent to the standard Wheeler DeWitt one. To reiterate, despite the profound differences between the quantum kinematics of LQC (on which our constructions are based) and that of the Wheeler DeWitt (WDW) framework, the *physical* Hilbert space representations are identical.

More interestingly, if we retain (iii) while suppressing (ii), we obtain (modulo some hitherto un- noticed technicalities which are relevant to WDW part of the APS work), well defined, regular evolution through an epoch where the size of the universe vanishes. Thus, as anticipated by APS the quantum bounce disappears due to the inavailability of feature (ii). Nevertheless, the singularity of the classical theory is resolved in that there is regular well defined evolution through the classically singular geometry. The physical observable of interest, namely the scalar field energy density, is always finite even in the classically singular region due to feature (iii). In this sense the singularity is still resolved even though there is no bounce. The details of the dynamics near the classically singular epoch are tied to the particular choice of Thiemann like procedure used to define the inverse scale factor operator.

The technicalities mentioned in the beginning of the previous paragraph are related to the issue of the validity of certain approximations used by APS to evaluate semiclassical behaviour for the Wheeler DeWitt quantization of the model. Recall that the scale factor operator acts by multiplication so that the wave function is a function of the scale factor . It turns out that the terms which APS neglect in their proposed semiclassical wave function significantly alter the behaviour of the wave function at large values of the logarithm of the scale factor. As a result, the Dirac observable corresponding to the scale factor operator at fixed value of the scalar field does not

have the APS wave function in its domain. However, (the mean value and fluctuation of) the operator corresponding to the logarithm of the scale factor at fixed ‘time’ (as measured by the scalar field) is well defined for this state. The secondary aim of this work is to point out the existence of these technicalities. The detailed calculations will be presented in a subsequent paper [9].

The layout of this paper is as follows. We provide a brief review of the model and its quantum kinematics in section 2. While several of the LQC constructions (see the references in [6]) were already standard prior to the seminal APS work, for convenience as well as to take advantage of some key APS insights we refer the reader to References [2, 3] for further details; indeed we shall lean heavily on those papers. In section 3, we show how to construct an LQC quantization without the introduction of curvature corrections. We use key ideas from the APS work [3]. In section 4, we construct the physical state space appropriate to the absence of (ii), using group averaging techniques. In section 5 we switch off both (ii) and (iii) and show that the resultant physical Hilbert space representation is identical to the Wheeler DeWitt one. We also point out the technicalities concerned with semiclassical analysis mentioned above. In section 6, we construct the representation obtained by switching off (ii) but retaining (iii) for the theory and show that the singularity is resolved. While we postpone an analysis of semiclassical states to a subsequent paper [9] (wherein we also fill the some of the lacunae in the semiclassical Wheeler DeWitt analysis of APS), our results in [9] support our statement of singularity resolution.

In section 7 we comment on the freedom in defining the inverse scale factor operator using Thiemann like procedures and argue that, given the interpretation of the operator, it is reasonable to incorporate a dependence on the fiducial cell size (see [2, 3]) so that the statement of singularity resolution is independent of the choice of fiducial cell. Section 8 contains a summary of our results and discusses open issues.

2 Brief review of classical theory and quantum kinematics

We provide a brief review of the classical Hamiltonian description of the model and its LQC quantum kinematics. We refer the reader to References [2, 3] for details. Our notation and conventions agree with those of [2, 3].

2.1 Classical Hamiltonian description

Since the spatial slice is non- compact and the fields are homogeneous, integrals over the slice diverge necessitating the choice of an elementary cell \mathcal{V} in the spatial slice which serves as the domain of integration. Fix a fiducial

metric ${}^0q_{ab}$, a set of co-triads, ${}^0\omega_a^i$ and triads ${}^0e_i^a$ which are compatible with, and orthonormal with respect to fiducial metric, and let V_0 be the volume of the fiducial cell with respect to the fiducial metric. The gravitational phase space variables are the connection A_a^i and the densitized triad E_i^a , and are parametrised as

$$A_a^i = cV_0^{-\frac{1}{3}} {}^0\omega_a^i \quad E_i^a = pV_0^{-\frac{2}{3}} {}^0e_i^a \quad (1)$$

with the symplectic structure

$$\{c, p\} = \frac{8\pi G\gamma}{3} \quad (2)$$

where γ is the Barbero- Immirzi parameter and G is Newton's constant. It is easy to see that the volume v of the elementary cell in the *physical* metric defined by E_i^a is

$$V := |p|^{\frac{3}{2}} \quad (3)$$

The massless scalar field ϕ and its conjugate momentum p_ϕ have Poisson bracket $\{\phi, p_\phi\} = 1$. The diffeomorphism and Gauss Law constraints vanish identically and the Hamiltonian constraint is

$$C = -\frac{6}{\gamma^2}c^2|p|^{\frac{1}{2}} + 8\pi G \frac{p_\phi^2}{|p|^{\frac{3}{2}}} \quad (4)$$

There are 4 degrees of freedom and a single constraint so that there are 2 true degrees of freedom which indicates the necessity of a choice of two independent Dirac observables.

Let $\vec{P} = (c, p, \phi, p_\phi)$ denote a point on the constraint surface. Since $\phi = \phi_0 = \text{constant}$ is a good gauge fixing, each gauge orbit can be labelled by its intersection with this gauge fixing slice in phase space. Let the gauge orbit through \vec{P} intersect $\phi = \phi_0$ at $\vec{P}_{\phi_0}(\vec{P}) = (c|_{\phi_0}, p|_{\phi_0}, \phi_0, p_\phi|_{\phi_0})$. Let $f(\vec{P})$ be any function on the constraint surface. Then $f(\vec{P}_{\phi_0}(\vec{P})) := f_{\phi_0}(\vec{P})$ is gauge invariant. By changing ϕ_0 we obtain a 1 parameter family of Dirac observables. These can be interpreted as describing the evolution of f_{ϕ_0} if we identify ϕ_0 with a choice of time.

Setting $f := p_\phi$, we have that $p_\phi|_{\phi_0}$ is a Dirac observable. Since $\{p_\phi, C\} = 0$, we have that $p_\phi|_{\phi_0} = p_\phi$. APS choose $p_\phi, p|_{\phi_0}$ as Dirac observables. It can be checked that $p|_{\phi_0}$ satisfies the equation:

$$\frac{dp|_{\phi_0}}{d\phi_0} = \pm \sqrt{16\pi G/3}p|_{\phi_0}. \quad (5)$$

The \pm signs correspond to the expanding and contracting branches. For the expanding branch equation (5) implies that starting from some non-vanishing $p_{\phi_0=\phi_*}$ at time ϕ_* , and evolving backwards we have

$$p|_{\phi_0 \rightarrow -\infty} \rightarrow 0 \quad (6)$$

at which point the size of the universe goes to zero and the matter density $\frac{p_\phi}{V_{\phi_0}}$ diverges (here we have used the notation above and set $f = V$ to define V_{ϕ_0}). This is the Big Bang singularity and every expanding classical solution originates from it.

We shall find it convenient to choose p_ϕ, x_{ϕ_0} as Dirac observables where x is an appropriately defined function of p (see equation (33)).

2.2 LQC quantum kinematics

The basic operators of LQC in the gravity sector are $\hat{e}^{i\lambda c}, \beta \in R$ and \hat{p} . Their action on eigen states of \hat{p} is

$$\hat{e}^{i\lambda c}|\mu\rangle = |\mu + \lambda\rangle \quad \hat{p}|\mu\rangle = \frac{8\pi\gamma l_P^2}{6}\mu|\mu\rangle \quad (7)$$

where $l_P^2 = G\hbar$ and $\mu \in R$. The Hilbert space \mathcal{H}_{kin}^{grav} is spanned by eigen states of μ and the inner product is defined through

$$\langle \mu_1 | \mu_2 \rangle = \delta_{\mu_1, \mu_2} \quad (8)$$

where $\delta_{\mu_1, \mu_2} = 1$ if $\mu_1 = \mu_2$ and vanishes otherwise. While $\hat{e}^{i\lambda c}$ are unitary operators, the above inner product does not endow them with enough continuity in λ for \hat{c} to be defined as an operator on \mathcal{H}_{kin}^{grav} . The matter operators are represented in the standard $L^2(R, d\phi)$ representation wherein $\hat{\phi}$ acts by multiplication and $\hat{p}_\phi := \frac{\hbar}{i} \frac{d}{d\phi}$.

The kinematic Hilbert space \mathcal{H}_{kin} for the model is just the product space $\mathcal{H}_{kin}^{grav} \otimes L^2(R, d\phi)$.

3 Quantization without curvature corrections

Since \hat{c} is not defineable on \mathcal{H}_{kin} , APS replace \hat{c} in the Hamiltonian constraint by $\frac{\hat{e}^{i\lambda c} - \hat{e}^{i\lambda c}}{2i\lambda}$ for small (but necessarily non-vanishing) λ . Since $\lambda \neq 0$, this amounts to the addition of the higher order curvature corrections (to the general relativistic expression of the Hamiltonian constraint) alluded to in (ii) of section 1. While λ was chosen to be a fixed number in [2], this was improved upon from a physical standpoint in [3] wherein λ was allowed to be operator valued and dependent on \hat{p} . The construction and well defined action of the operator $\hat{e}^{i\lambda c}$ with λ being an operator valued function of \hat{p} , was one of the key insights of APS [3]. We shall use this key insight of APS in conjunction with the group averaging technique [8] to construct a quantization of the model without curvature corrections.

First, note that the Hamiltonian constraint C may be written as

$$C = -C_+ C_- \quad (9)$$

where

$$C_{\pm} = -\sqrt{\frac{6}{\gamma^2}} c |p|^{\frac{1}{4}} \pm \sqrt{8\pi G} \frac{p_{\phi}}{|p|^{\frac{3}{4}}} \quad (10)$$

so that the vanishing of C is equivalent to that of C_+ or C_- or both. We shall construct the physical Hilbert space as the union of the kernels of \hat{C}_{\pm} . However, since it is not possible to define \hat{C}_{\pm} as operators, we shall first define their exponentials, $e^{i\lambda C_{\pm}}$ as unitary operators and then find the physical state space by group averaging the action of these unitary operators.

We shall work in the μ representation. We start with the following heuristics. Following APS we define \hat{C}_{\pm} by $\hat{c} = 2i \frac{d}{d\mu}$ and $\hat{p} = \frac{8\pi G l_P^2}{6} \mu$ (this is heuristic since \hat{c} is not a well defined operator on \mathcal{H}_{kin}). In anticipation of a Thiemann like definition of the operator $|p|^{-\frac{3}{2}}$ (which we assume is diagonal in the μ representation as in [2, 3]), we set

$$|p|^{-\frac{3}{2}} = \left(\frac{4\pi}{3}\gamma l_P^2\right)^{-\frac{3}{2}} B(\mu) \quad (11)$$

It is useful to define

$$\tilde{C}_{\pm} := \left(4\left(\frac{3\pi l_P^2}{\gamma^3}\right)^{\frac{1}{4}}\right)^{-1} C_{\pm}. \quad (12)$$

Motivated by the considerations in the previous paragraph, we define the action of the operators $e^{i\alpha \hat{C}_{\pm}}$ in the μ representation by

$$e^{i\alpha \hat{C}_{\pm}} = \exp \alpha \left(|\mu|^{\frac{1}{4}} \frac{d}{d\mu} \pm i \frac{B^{1/2}(\mu) \hat{p}_{\phi}}{\sqrt{\frac{16\pi G \hbar^2}{3}}} \right), \quad (13)$$

where $\alpha \in R$. Again, following the ideas of APS we define

$$l := \frac{4}{3} \text{sgn}(\mu) |\mu|^{\frac{3}{4}}. \quad (14)$$

Note that l is an invertible function of μ . From (14) it follows that

$$|\mu|^{\frac{1}{4}} \frac{d}{d\mu} = \frac{d}{dl}. \quad (15)$$

With this change of variables it follows that

$$e^{i\alpha \hat{C}_{\pm}} = \exp \alpha \left(\frac{d}{dl} \pm i \frac{B^{1/2}(\mu) \hat{p}_{\phi}}{\sqrt{\frac{16\pi G \hbar^2}{3}}} \right) \quad (16)$$

$$= e^{\mp i \frac{x(l) \hat{p}_{\phi}}{\sqrt{\frac{16\pi G \hbar^2}{3}}}} e^{\alpha \frac{d}{dl}} e^{\pm i \frac{x(l) \hat{p}_{\phi}}{\sqrt{\frac{16\pi G \hbar^2}{3}}}}. \quad (17)$$

Here $x(l)$ is defined as

$$x(l) = \int_L^l B^{1/2}(\mu(\bar{l})) d\bar{l} \quad (18)$$

with some (fixed) choice of lower limit of integration L .

Since μ is an invertible function of l , it is convenient to label the eigenstates of \hat{p} by l rather than μ so that

$$\hat{p}|l\rangle := \frac{8\pi\gamma l_P^2}{6}\mu(l)|l\rangle = \text{sgn}(l)\frac{3}{4}|l|^{\frac{4}{3}}|l\rangle \quad (19)$$

$$\langle l_1|l_2\rangle = \delta_{l_1,l_2} \quad (20)$$

Thus any state $|\psi\rangle \in \mathcal{H}_{kin}$ can be written as

$$|\psi\rangle = \sum_l \int d\phi \psi(l, \phi) |l\rangle \otimes |\phi\rangle. \quad (21)$$

In this l -representation, it follows from the inner product (20) and the inner product on $L^2(R, d\phi)$ that the inner product between two states $|\psi_1\rangle, |\psi_2\rangle$ is given by

$$\langle \psi_1 | \psi_2 \rangle = \sum_l \int \psi_1^*(l, \phi) \psi_2(l, \phi) \quad (22)$$

From (17) it follows that the action of the exponentiated constraint operators $e^{i\alpha\tilde{C}_\pm}$ on the state $|\Psi\rangle$ defined by equation (21) is defined to be

$$e^{i\alpha\hat{\tilde{C}}_\pm} |\psi\rangle = \sum_l \int d\phi \psi(l, \phi \pm \beta_0(x(l) - x(l - \alpha))) |l - \alpha\rangle \otimes |\phi\rangle \quad (23)$$

where we have defined β_0 by

$$\beta_0 := (\sqrt{\frac{16\pi G}{3}})^{-1} \quad (24)$$

It can be checked that this action is unitary in the inner product (22) on \mathcal{H}_{kin} .

Thus, motivated by the ideas of APS [3], we have constructed the well defined unitary operators $e^{i\alpha\hat{\tilde{C}}_\pm}$ on \mathcal{H}_{kin} without recourse to any curvature corrections. In the next section we construct the kernel of the constraints C_\pm (or, equivalently \tilde{C}_\pm (see equation (12)) by group averaging the action of the operators defined in equation (23). As mentioned above, the kernel of the Hamiltonian constraint will be identified with the union of the kernels of C_+ and C_- .

4 Group Averaging and the Physical Hilbert Space

We start with a brief review of the group averaging technique. Only gauge invariant states are physical so that physical states Ψ must satisfy the condition $\hat{U}(g)\Psi = \Psi$, $\forall g$ where $\hat{U}(g)$ is the unitary operator which implements the finite gauge transformation denoted by g . A formal solution to this condition is to fix some $|\psi\rangle \in \mathcal{H}_{kin}$ and set $\Psi = \sum |\psi'\rangle$ where the sum is over all distinct $|\psi'\rangle$ which are gauge related to $|\psi\rangle$. A mathematically precise implementation of this idea places the gauge invariant states in the dual representation (corresponding to a formal sum over bras rather than kets) and goes by the name of Group Averaging. The “Group” is that of gauge transformations and the “Averaging” corresponds to the construction of a gauge invariant state from a kinematical one by giving meaning to the formal sum over gauge related states. Specifically (for details see Reference [8]), the physical Hilbert space can be constructed if there exists an anti-linear map η from a dense subspace \mathcal{D} of the kinematical Hilbert space \mathcal{H}_{kin} , to its algebraic dual \mathcal{D}^* , subject to certain requirements. The algebraic dual of \mathcal{D} is defined to be the space of linear mappings from \mathcal{D} to the complex numbers. The requirements which η needs to satisfy are as follows. Let $|\psi_1\rangle, |\psi_2\rangle \in \mathcal{D}$, let \hat{A} be a (strong) Dirac observable of interest and let g be a gauge transformation with $\hat{U}(g)$ being its unitary implementation on \mathcal{H}_{kin} . Let $\eta(|\psi_1\rangle) \in \mathcal{D}^*$ denote the image of $|\psi_1\rangle$ by η and let $\eta(|\psi_1\rangle)[|\psi_2\rangle]$ denote the complex number obtained by the action of $\eta(|\psi_1\rangle)$ on $|\psi_2\rangle$. Then for all $|\psi_1\rangle, |\psi_2\rangle, \hat{A}, g$ we require that

- (1) $\eta(|\psi_1\rangle)[|\psi_2\rangle] = \eta(|\psi_1\rangle)[\hat{U}(g)|\psi_2\rangle]$
- (2) $\eta(|\psi_1\rangle)[|\psi_2\rangle] = (\eta(|\psi_2\rangle)[|\psi_1\rangle])^*, \eta(|\psi_1\rangle)[|\psi_1\rangle] \geq 0$.
- (3) $\eta(|\psi_1\rangle)[\hat{A}|\psi_2\rangle] = \eta(\hat{A}^\dagger|\psi_1\rangle)[|\psi_2\rangle]$.

It turns out that typically (, and in the case of interest here,) we may indeed write $\eta(|\psi\rangle) = \sum \langle \psi' |$ where the sum is over all distinct $\langle \psi' |$ which are gauge related to $\langle \psi |$. As we shall see only a finite number of terms in the sum have a non-vanishing kinematical inner product with any state in \mathcal{D} so that $\eta(|\psi\rangle)$ (with its action defined on states in \mathcal{D} in the obvious, natural way suggested by its representation by the sum above) indeed lies in the algebraic dual space. An inner product on the space $\eta(\mathcal{D})$ can be defined through

$$\langle \eta(|\psi_1\rangle), \eta(|\psi_2\rangle) \rangle = \eta(|\psi_1\rangle)[|\psi_2\rangle]. \quad (25)$$

The requirements (1), (2) ensure that the right hand side of the above equation defines a positive, hermitian inner product. The completion of $\eta(\mathcal{D})$ in this inner product is the physical Hilbert space. It can be checked that the condition (3) ensures that the above inner product automatically implements the adjointness conditions on the Dirac observables (which act by

dual action on \mathcal{D}^*)¹ if these conditions are implemented on \mathcal{H}_{kin} .

As mentioned in section 3 our strategy is to construct the kernel of the Hamiltonian constraint as the union of the + and -- sector kernels. Accordingly, in section 4.1 we define the group averaging maps η^\pm corresponding to the group averaging with respect to $e^{-i\alpha\tilde{C}_\pm}$ and construct the corresponding physical Hilbert spaces \mathcal{H}_{phys}^\pm .

In section 4.2 we construct the Dirac observables of the theory. In section 4.3 we identify the positive and negative frequency eigen states of the Dirac observable \hat{p}_ϕ within each sector \mathcal{H}_{phys}^\pm . Denote the positive frequency subspaces by \mathcal{H}_{+phys}^\pm . As in the APS work, we shall restrict attention to these positive frequency subspaces. The space of positive frequency physical states is the union of \mathcal{H}_{+phys}^+ and \mathcal{H}_{+phys}^- . While group averaging automatically provides the inner product between states within each sector \mathcal{H}_{phys}^\pm , it does not specify the inner product between a state in \mathcal{H}_{phys}^+ and one in \mathcal{H}_{phys}^- . In section 4.4 we show that the positive frequency subspaces of \mathcal{H}_{phys}^+ and \mathcal{H}_{phys}^- must be mutually orthogonal. Thus the positive frequency physical Hilbert space of the model, \mathcal{H}_{+phys} , is the union of its two mutually orthogonal positive frequency subspaces \mathcal{H}_{+phys}^+ and \mathcal{H}_{+phys}^- .² Finally, in section 4.5 we show that the representation on \mathcal{H}_{+phys} is isomorphic to an $L^2(R, dx)$ representation.

4.1 Construction of \mathcal{H}_{phys}^\pm by group averaging.

Consider states of the form

$$|\psi\rangle = \int d\phi \psi(\phi) |l\rangle \otimes |\phi\rangle \quad (26)$$

where $\psi(\phi)$ is smooth and normalizable in $L^2(R, d\phi)$. Clearly the finite span of such states defines a dense set $\mathcal{D} \subset \mathcal{H}_{kin}$. Let \mathcal{D}^* be its algebraic dual. Define the group averaging maps η^\pm from \mathcal{D} to \mathcal{D}^* through

$$\eta^\pm(|\psi\rangle) := \sum_\alpha \langle \psi | e^{-i\alpha\tilde{C}_\pm} \quad (27)$$

where the formal sum is over all $\alpha \in R$ and the right hand side is interpreted as an element of \mathcal{D}^* in the usual way [8]. For ease of notation in what follows, we set $l = l_0$ in (26) so that

$$|\psi\rangle := \int d\phi \psi(\phi) |l_0\rangle \otimes |\phi\rangle. \quad (28)$$

¹Given $\Psi \in \mathcal{D}^*$, $|\psi\rangle \in \mathcal{D}$ and \hat{A} such that $\hat{A}^\dagger|\psi\rangle \in \mathcal{D}$, define $\hat{A}\Psi$ through $\hat{A}\Psi[|\psi\rangle] := \Psi[\hat{A}^\dagger|\psi\rangle]$. This is the dual action.

²Similar arguments show that the negative frequency subspaces, \mathcal{H}_{-phys}^\pm of \mathcal{H}_{phys}^\pm are mutually orthogonal. Their union, \mathcal{H}_{-phys} , is the negative frequency physical Hilbert space of the model. Note that if we wish to work with both positive and negative frequency states, such states must be mutually orthogonal to ensure hermiticity of the Dirac observable \hat{p}_ϕ .

Then from (23), (27), (28) the action of η_{\pm} on $|\psi\rangle$ evaluates to

$$\eta^{\pm}(|\psi\rangle) = \sum_{\alpha} \int d\phi \psi^*(\phi \pm \beta_0(x(l_0) - x(l_0 - \alpha))) \langle l_0 - \alpha | \otimes \langle \phi| \quad (29)$$

$$= \sum_l \int d\phi \psi^*(\phi \pm \beta_0(x(l_0) - x(l))) \langle l | \otimes \langle \phi|. \quad (30)$$

where, in the second line, the sum is over all $l \in R$.

It can be checked that, for any $\lambda \in R$,

$$\eta^{\pm}(e^{i\lambda\hat{C}^{\pm}}|\psi\rangle) = \eta^{\pm}(|\psi\rangle). \quad (31)$$

Since the orbit of $\langle l_0 |$ under the averaging procedure is $\{\langle l |, l \in R\}$, ³ equation (31) implies that we may, without loss of generality, generate a basis for the physical state space by averaging over states of the form (28) with l_0 fixed once and for all. Next, consider the states $|\psi_1\rangle, |\psi_2\rangle$ of the form (31) with $\psi(\phi) = \psi_1(\phi), \psi_2(\phi)$ respectively. The inner product between the corresponding physical states obtained by group averaging, $(\eta^{\pm}(|\psi_1\rangle), \eta^{\pm}(|\psi_2\rangle))$, is defined as $(\eta^{\pm}(|\psi_1\rangle), \eta^{\pm}(|\psi_2\rangle)) := \eta^{\pm}(|\psi_2\rangle)[|\psi_1\rangle]$ where the $\eta^{\pm}(|\psi_2\rangle)[|\psi_1\rangle]$ denotes the natural action of elements of \mathcal{D}^* on elements of \mathcal{D} [8]. From (30) this evaluates to

$$(\eta^{\pm}(|\psi_1\rangle), \eta^{\pm}(|\psi_2\rangle)) = \int d\phi \psi_2^*(\phi) \psi_1(\phi) \quad (32)$$

which is clearly positive definite. ⁴

The completion of $\eta_{\pm}(\mathcal{D})$ in the inner product (32) yields the physical Hilbert spaces \mathcal{H}_{phys}^{\pm} .

4.2 The Dirac Observables

Recall from section 2 that \hat{p}_{ϕ} is one of our Dirac observables. It is straightforward to check that \hat{p}_{ϕ} commutes with $e^{i\alpha\hat{C}^{\pm}}$ as well as with the averaging maps η_{\pm} . Hence [8] it's kinematic self adjointness translates to self adjointness on the physical Hilbert spaces \mathcal{H}_{phys}^{\pm} .

Next recall from (14), (18) that $x := x(l) = x(l(\mu))$. Since the eigenvalues of \hat{p} are $\frac{8\pi\gamma l_P^2}{6}\mu$, we define

$$\hat{x} = x(l(\frac{\hat{p}}{8\pi\gamma l_P^2})) =: f(\hat{p}). \quad (33)$$

³ This is not strictly correct. As we shall see in section 6, this depends on the behaviour of $x(l)$. The attendant subtleties will be dealt with in section 6.

⁴One may also attempt to define the averaging map with respect to the averaging measure $\int da$. If one does this with the same choice of \mathcal{D} as above, one finds that all of \mathcal{D} is in the kernel of the group averaging maps or, equivalently, the physical inner product is completely degenerate.

Using the notation of section 2.1, we choose $f(p|\hat{\phi}_0) = \hat{x}_{\phi_0}$ as our second Dirac observable.

In order to represent this operator, it is useful to examine its classical correspondent, x_{ϕ_0} . To evaluate x_{ϕ_0} at any point on the constraint surface we first map the point in question via a gauge transformation to its gauge related image on the gauge fixing slice $\phi = \phi_0$ and then evaluate the function x there. The constraint surface splits (modulo a set of measure zero) into + and - sectors defined by $C_+ = 0, C_- \neq 0$ and $C_- = 0, C_+ \neq 0$ respectively. Denote the restriction of the function x_{ϕ_0} to the \pm sector by $x_{\phi_0}^\pm$. Correspondingly, in quantum theory, we define the action of $\hat{x}_{\phi_0}^\pm$ on an eigen state of $\hat{\phi}$ by first mapping the state to the eigen state with eigenvalue ϕ_0 by an appropriate gauge transformation of the form $e^{i\alpha\tilde{C}_\pm}$, acting with \hat{x} and then performing the inverse gauge transformation.

Hence the action of the operators $\hat{x}_{\phi_0}^\pm$ relevant to the physical Hilbert spaces \mathcal{H}_{phys}^\pm is obtained as follows. From (23),

$$e^{i\alpha\tilde{C}_\pm}|l\rangle \otimes |\phi\rangle = |l - \alpha\rangle \otimes |\phi \pm \beta_0(x(l) - x(l - \alpha))\rangle, \quad (34)$$

where α is chosen so that $\phi_0 = \phi \mp \beta_0(x(l) - x(l - \alpha))$ which implies that $x(l - \alpha) = x(l) \pm (\phi_0 - \phi)$. It follows that

$$\hat{x}_{\phi_0}^\pm|l\rangle \otimes |\phi\rangle = (x(l) \pm \frac{\phi - \phi_0}{\beta_0})|l\rangle \otimes |\phi\rangle, \quad (35)$$

so that

$$\hat{x}_{\phi_0}(\eta^\pm(|\psi\rangle)) := \hat{x}_{\phi_0}^\pm(\eta^\pm(|\psi\rangle)) \quad (36)$$

$$= \sum_l \int d\phi \langle l | \otimes \langle \phi | \chi^*(\phi \pm \beta_0(x(l_0) - x(l))), \quad (37)$$

where $|\psi\rangle$ is given by equation (28) and

$$\begin{aligned} \chi(\phi \pm \beta_0(x(l_0) - x(l))) &:= \mp \beta_0^{-1}\{\phi \pm \beta_0(x(l_0) - x(l)) - (\phi_0 \pm \beta_0 x(l_0))\} \\ &\quad \psi(\phi \pm \beta_0(x(l_0) - x(l))) \end{aligned} \quad (38)$$

It can be verified that $[\hat{x}_{\phi_0}, e^{i\lambda\tilde{C}_\pm}] = 0, \lambda \in R$, that $[\hat{x}_{\phi_0}, \eta^\pm] = 0$ and that \hat{x}_{ϕ_0} is a self adjoint operator on \mathcal{H}_{phys}^\pm .

4.3 Eigen functions of \hat{p}_ϕ in \mathcal{H}_{phys}^\pm .

Since \hat{p}_ϕ commutes with the averaging maps η_\pm it follows that group averages of kinematic eigen states of \hat{p}_ϕ are eigen states of \hat{p}_ϕ with unchanged eigen values. The (positive and negative) frequency kinematic eigen states of \hat{p}_ϕ are

$$\psi_{\pm\omega}(\phi) = e^{\pm i\omega\phi} \quad \omega > 0. \quad (39)$$

We shall restrict attention to the positive frequency states. From equation (30) these states under group averaging yield (upto an unimportant constant phase factor which we drop),

$$\eta^\pm(|\psi_\omega\rangle) := \sum_l \int d\phi e^{-i\omega\phi} e^{\pm i\beta_0\omega x(l)} \langle l| \otimes \langle \phi|. \quad (40)$$

The physical positive frequency eigenstates, $\eta^\pm(|\psi_\omega\rangle)$, form a spanning set in the positive frequency physical Hilbert spaces \mathcal{H}_+^\pm . This follows from the fact that the kinematic positive frequency eigenstates, $|\psi_\omega\rangle = \int d\phi e^{i\omega\phi} |l\rangle \otimes |\phi\rangle$ span the positive frequency part of the kinematic Hilbert space.

Finally, note that from (32) it follows that

$$(\eta^\pm(|\psi_{\omega_1}\rangle), \eta^\pm(|\psi_{\omega_2}\rangle)) = 2\pi\delta(\omega_1, \omega_2) \quad (41)$$

where $\delta(\omega_1, \omega_2)$ is the Dirac delta function.

4.4 Mutual orthogonality of \mathcal{H}_{+phys}^+ , \mathcal{H}_{+phys}^- .

Our strategy is as follows. The phase space function, F , defined by

$$F = -\left(\frac{6}{8\pi G\gamma^2}\right)^{1/2} c|p| \quad (42)$$

is a (weak) Dirac observable. We shall represent \hat{F} as an operator on \mathcal{H}_{+phys}^\pm and show that the positive frequency eigen functions $\eta^\pm(|\psi_\omega\rangle)$ are also eigen functions of \hat{F} with eigen values $\mp\omega$. In order that \hat{F} be represented as a self adjoint operator, its eigen spaces with distinct eigenvalues must be orthogonal. The mutual orthogonality of \mathcal{H}_{+phys}^\pm follows.

From considerations similar to those of section 3, we represent the operator $e^{\frac{i\hat{\beta}_0\lambda}{\hbar}\hat{F}}$ on states $|\psi\rangle$ of the form (28) by

$$e^{\frac{i\hat{\beta}_0\lambda}{\hbar}\hat{F}}|\psi\rangle = \int d\phi \psi(\phi) |x^{-1}[x(l_0) - \lambda]\rangle \otimes |\psi\rangle. \quad (43)$$

This follows from the (heuristic) following choice of representation for \hat{F} in the l - representation:

$$\hat{F} = -\left(\frac{6}{8\pi G\gamma^2}\right)^{1/2} c|\hat{p}|^{1/4} \frac{1}{|\hat{p}|^{-3/4}} = -i\hbar(\beta_0)^{-1} B^{-1/2}(\mu) \frac{d}{dl} = -i\hbar(\beta_0)^{-1} \frac{d}{dx(l)}. \quad (44)$$

Again, we shall ignore the subtleties indicated in Footnote 3 and assume that $x(l)$ is an invertible function of l . We shall clarify these subtleties in sections 5 and 6.

It is straightforward to check that, under the assumption of invertibility of $x(l)$, $e^{\frac{i\hat{\beta}_0\lambda}{\hbar}\hat{F}}$ is a unitary operator. Next, note that $e^{\frac{i\hat{\beta}_0\lambda}{\hbar}\hat{F}}$ commutes with

the averaging maps η^\pm . To see this, note that equations (28),(30) and (43) imply that

$$\eta^\pm(e^{\frac{i\beta_0\lambda}{\hbar}\hat{F}}|\psi\rangle) = \sum_l \int d\phi \psi^*(\phi \pm \beta_0(x(l_0) - (x(l) + \lambda))) \langle l| \otimes \langle \phi|. \quad (45)$$

On the other hand, we have that

$$\begin{aligned} e^{\frac{i\beta_0\lambda}{\hbar}\hat{F}}\eta^\pm(|\psi\rangle) &= \sum_l \int d\phi \psi^*(\phi \pm \beta_0(x(l_0) - x(l))) \langle l| \otimes \langle \phi| e^{-\frac{i\lambda}{\beta_0\hbar}\hat{F}} \\ &= \sum_l \int d\phi \psi^*(\phi \pm \beta_0(x(l_0) - x(l))) \langle x^{-1}[x(l) - \lambda]| \otimes \langle \phi| \quad (46) \\ &= \sum_{\bar{l}} \int d\phi \psi^*(\phi \pm \beta_0(x(l_0) - (x(\bar{l}) + \lambda))) \langle \bar{l}| \otimes \langle \phi|, \quad (47) \end{aligned}$$

where in the last line we have set $\bar{l} = x^{-1}(x(l) - \lambda)$. The assumed invertibility of $x(l)$ ensures that (47) is the same as the right hand side of (45). Thus, $e^{\frac{i\beta_0\lambda}{\hbar}\hat{F}}$ commutes with the averaging maps and defines an operator on the physical Hilbert spaces \mathcal{H}^\pm .

Next, note from (45) that

$$\lim_{\lambda \rightarrow 0} \frac{e^{\frac{i(\beta_0\lambda)}{\hbar}\hat{F}} - 1}{\lambda} \eta^\pm(|\psi\rangle) = \sum_l \int d\phi \left[\frac{d}{dx(l)} \psi^*(\phi \pm \beta_0(x(l_0) - x(l))) \right] \langle l| \otimes \langle \phi| \quad (48)$$

Clearly, this allows us to define the action of the operator \hat{F} on physical states through the action

$$\hat{F}\eta^\pm(|\psi\rangle) = \sum_l \int \left[(i\hbar(\beta_0)^{-1} \frac{d}{dx(l)}) \psi^*(\phi \pm \beta_0(x(l_0) - x(l))) \right] \langle l| \otimes \langle \phi| \quad (49)$$

With this definition of \hat{F} it is easy to see that

$$\hat{F}\eta^\pm(|\psi_\omega\rangle) = \mp\omega\eta^\pm(|\psi_\omega\rangle). \quad (50)$$

Hermiticity then requires the mutual orthogonality of \mathcal{H}_{+phys}^+ and \mathcal{H}_{+phys}^- .

4.5 Isomorphism with an $L^2(R, dx)$ representation.

The representation we have constructed through group averaging is an anti-representation due to the dual action of operators on \mathcal{D}^* . Hence its conjugate representation is a true representation. The state conjugate to that in (30) is characterised by the wave function $\psi(\phi \pm \beta_0(x(l_0) - x(l)))$. Henceforth, with no loss of generality, we shall set $l_0 = L$ so that $x(l_0) = 0$ (see (18)). Thus, wave functions in the conjugate Hilbert spaces $\mathcal{H}_{phys}^{*\pm}$ are of the form

$$\psi^\pm(l, \phi) = \psi^\pm(\phi \mp \beta_0 x(l)). \quad (51)$$

Clearly, the operator \hat{p}_ϕ acts as

$$\hat{p}_\phi \psi^\pm(l, \phi) = \frac{\hbar}{i} \frac{d}{d\phi} \psi^\pm(l, \phi). \quad (52)$$

The positive frequency eigenstates are

$$\psi_\omega^\pm(l, \phi) = e^{i\omega\phi} e^{\mp\beta_0\omega x(l)}. \quad (53)$$

For the remainder of this section we shall restrict attention to positive frequency wave functions. From equation (38) we have that

$$\beta_0 \hat{x}_{\phi_0} \psi_\omega^\pm(l, \phi) = [\mp(\phi \mp \beta_0 x(l)) \pm \phi_0] \psi_\omega^\pm(l, \phi). \quad (54)$$

Any state in the positive frequency Hilbert space $\mathcal{H}_+^{*\pm}$ can be expanded as

$$\psi^\pm(l, \phi) = \int_0^\infty d\omega f_\pm(\omega) \psi_\omega^\pm(l, \phi). \quad (55)$$

It is easy to check that

$$\begin{aligned} \beta_0 \hat{x}_{\phi_0} \psi^\pm(l, \phi) &= \mp i \int_0^\infty d\omega \frac{df_\pm(\omega)}{d\omega} \psi_\omega^\pm(l, \phi) \\ &\quad \mp i(f_\pm(0) - f_\pm(\infty)) \pm \phi_0 \psi^\pm(l, \phi). \end{aligned} \quad (56)$$

Hence \hat{x}_{ϕ_0} is a well defined operator if $f_\pm(0) = f_\pm(\infty) = 0$. For arbitrary powers of \hat{x}_{ϕ_0} to be (densely) defined we require that $f_\pm(\omega)$ and all its derivatives vanish at zero and infinity i.e. we require that for all positive integers n ,

$$f_\pm(\omega), \frac{d^n}{d\omega^n} f_\pm(\omega) \rightarrow 0 \text{ as } \omega \rightarrow 0, \infty. \quad (57)$$

On this dense domain, $\beta_0 \hat{x}_{\phi_0}$ acts as

$$\beta_0 \hat{x}_{\phi_0} \psi^\pm(l, \phi) = \mp i \int_0^\infty d\omega \frac{df_\pm(\omega)}{d\omega} \psi_\omega^\pm(l, \phi) \pm \phi_0 \psi^\pm(l, \phi). \quad (58)$$

Rewrite $\psi^-(l, \phi)$ as

$$\psi^-(l, \phi) = \int_{-\infty}^0 d\omega f_-(-\omega) e^{i|\omega|\phi} e^{-i\omega\beta_0 x} \quad (59)$$

so that $\beta_0 \hat{x}_{\phi_0}$ acts as

$$\beta_0 \hat{x}_{\phi_0} \psi^-(l, \phi) = -i \int_{-\infty}^0 d\omega \frac{d}{d\omega} f_-(-\omega) e^{i|\omega|\phi} e^{-i\omega\beta_0 x} - \phi_0 \psi^-(l, \phi). \quad (60)$$

The inner product on $\mathcal{H}_+^* = \mathcal{H}_+^{*+} \oplus \mathcal{H}_+^{*-}$ is defined through

$$(\psi_\omega^\pm, \psi_{\omega'}^\pm) = 2\pi\delta(\omega, \omega') \quad (\psi_\omega^+, \psi_{\omega'}^-) = 0, \quad \omega, \omega' > 0, \quad (61)$$

which yields the inner product between any $\psi_1(l, \phi), \psi_2(l, \phi) \in \mathcal{H}_{+phys}^*$ (in obvious notation):

$$(\psi_1, \psi_2) = 2\pi \left[\int_0^\infty f_{1+}^*(\omega) f_{2+}(\omega) d\omega + \int_{-\infty}^0 f_{1-}^*(-\omega) f_{2-}(-\omega) d\omega \right] \quad (62)$$

where

$$\psi_i(l, \phi) = \psi_i^+(l, \phi) \oplus \psi_i^-(l, \phi), \quad i = 1, 2. \quad (63)$$

Equations (52), (58), (60), (62) imply that the representation on \mathcal{H}_{+phys}^* is unitarily equivalent to an $L^2(R, dx)$ representation. Specifically, let U be a linear map from \mathcal{H}_{+phys}^* to $L^2(R, dx)$ generated by its action on the positive frequency eigenstates as follows.

$$U(\psi_{\frac{|k|}{\beta_0}}^+(l, \phi)) = \beta_0^{-\frac{1}{2}} e^{i\frac{|k|}{\beta_0}\phi} e^{-ikx}, \quad k > 0, \quad (64)$$

$$U(\psi_{\frac{|k|}{\beta_0}}^-(l, \phi)) = \beta_0^{-\frac{1}{2}} e^{i\frac{|k|}{\beta_0}\phi} e^{-ikx}, \quad k < 0. \quad (65)$$

This implies that

$$U(\psi(l, \phi)) =: \Psi(x, \phi) = \int_{-\infty}^\infty dk f(k) e^{i\frac{|k|}{\beta_0}\phi} e^{-ikx} \quad (66)$$

$$\begin{aligned} f(k) &= \beta_0^{-\frac{1}{2}} f_+(\frac{k}{\beta_0}), \quad k > 0 \\ &= \beta_0^{-\frac{1}{2}} f_-(\frac{-k}{\beta_0}), \quad k < 0. \end{aligned} \quad (67)$$

The inner product on $L^2(R, dx)$ is

$$(\Psi_1(x, \phi), \Psi_2(x, \phi)) = \int_{-\infty}^\infty dx \Psi_1^*(x, \phi) \Psi_2(x, \phi). \quad (68)$$

It is easy to check that U is a unitary map and that $\hat{p}_\phi, \hat{x}_{\phi_0}$ act on states in $L^2(R, dx)$ via U as

$$\hat{p}_\phi \Psi(x, \phi) = \frac{\hbar}{i} \frac{d}{d\phi} \Psi(x, \phi) \quad (69)$$

$$\hat{x}_{\phi_0} \Psi(x, \phi) = \int_{-\infty}^\infty dk \left(\frac{1}{i} \frac{d}{dk} + \frac{k}{\beta_0 |k|} \phi_0 \right) f(k) e^{i\frac{|k|}{\beta_0}\phi} e^{-ikx}, \quad (70)$$

where in (70) $f(k)$ satisfies the appropriate conditions implied by equation (57).

5 The physical state space in the absence of Thiemann-like inverse triad definitions.

Set $B(\mu) = |\mu|^{-3/4}$. Equation (14) implies that $B^{1/2}(\mu(l)) = \frac{4}{3}|l|^{-1}$. Set $L > 0$ in equation (18). Then we have that

$$\begin{aligned} x(l) &= \frac{4}{3} \int_L^l |\bar{l}|^{-1} = \frac{4}{3} \ln \frac{l}{L} \\ &= \infty \text{ for } l \leq 0 \end{aligned} \quad (71)$$

The square integrability of $\psi(\phi)$ in (28) implies that $\psi(\phi \pm (x(l_0) - x(l))) = 0$ for $l \leq 0$. Thus for $l_0 > 0$ the orbit of $\langle l_0 |$ under group averaging is effectively $\{\langle l |, l > 0\}$. To access $l < 0$ we must choose $l_0 < 0$. This implies that \mathcal{H}_{phys} splits up into 2 orthogonal sectors, $\mathcal{H}_{>phys}, \mathcal{H}_{<phys}$, one obtained for $l_0 > 0$ and the other from $l_0 < 0$ (orthogonality follows from the inner product defined through group averaging).

Accordingly set $l_0 = L = 1$ to obtain $\mathcal{H}_{>phys}^*$ and $l_0 = L = -1$ to obtain $\mathcal{H}_{<phys}^*$. It is then straightforward to see that the considerations of sections 4.2- 4.4 apply to each sector $\mathcal{H}_{>phys}^*, \mathcal{H}_{<phys}^*$, individually by virtue of the invertibility of $x(l)$ in each sector. We shall use obvious notation with subscripts $>, <$ referring to the appropriate sector. Thus, we have that

$$x(l) := x_{>}(l) = \ln |l|, l > 0 \quad (72)$$

$$x(l) := x_{<}(l) = -\ln |l|, l < 0 \quad (73)$$

so that $x_{>}, x_{<}$ are invertible functions of l for $l > 0, l < 0$.

The positive frequency eigenfunctions now acquire a 4-fold (rather than 2-fold) degeneracy. These eigenfunctions, in the l, ϕ representation, are:

$$\begin{aligned} \psi_{>\omega}^\pm(l, \phi) &= e^{i\omega\phi} e^{\mp\beta_0\omega x_{>}(l)}, \quad l > 0, \\ &= 0, \quad l \leq 0 \end{aligned} \quad (74)$$

$$\begin{aligned} \psi_{<\omega}^\pm(l, \phi) &= e^{i\omega\phi} e^{\mp\beta_0\omega x_{<}(l)}, \quad l < 0, \\ &= 0, \quad l \geq 0. \end{aligned} \quad (75)$$

The representation on \mathcal{H}_{+phys}^* is now unitarily equivalent to one on $L^2(R, dx_{>}) \oplus L^2(R, dx_{<})$. Replacing $x_{>}, x_{<}$ by $x_{>}(l), x_{<}(l)$ it is straightforward to see that

$$L^2(R, dx_{>}) \oplus L^2(R, dx_{<}) = L^2(R, |l|^{-1} dl). \quad (76)$$

The explicit unitary mapping is as follows. A positive frequency state $\psi(l, \phi) \in \mathcal{H}_{+phys}^*$ is characterised by its mode functions $f_{>\pm}(\omega), f_{<\pm}(\omega), \omega > 0$. Define the linear map $U, U : \mathcal{H}_{+phys}^* \rightarrow L^2(R, |l|^{-1} dl)$ as follows.

$$U(\psi(l, \phi)) =: \Psi(x, \phi) = \int_{-\infty}^{\infty} dk f_{>}(k) e^{i\frac{|k|}{\beta_0}\phi} e^{-ik \ln |l|}, \quad l > 0, \quad (77)$$

$$= \int_{-\infty}^{\infty} dk f_{<}(k) e^{i\frac{|k|}{\beta_0}\phi} e^{ik \ln |l|}, \quad l < 0, \quad (78)$$

where the mode coefficients $f_>(k), f_<(k)$ are related to $f_{>\pm}(\omega), f_{<\pm}(\omega)$ through the analogs of equation (67) i.e. $f(k), f_\pm(\omega)$ in that equation are replaced by $f_>(k), f_{>\pm}(\omega)$ and $f_<(k), f_{<\pm}(\omega)$.

The inner product between $\Psi_1(l, \phi), \Psi_2(l, \phi) \in L^2(R, |l|^{-1}dl)$ is

$$(\Psi_1(x, \phi), \Psi_2(x, \phi)) = \int_{-\infty}^{\infty} \frac{dl}{|l|} \Psi_1^*(l, \phi) \Psi_2(l, \phi). \quad (79)$$

It is straightforward to check that U is a unitary map and that $\hat{p}_\phi, \hat{x}_{\phi_0}$ act on states in $L^2(R, |l|^{-1}dl)$ via U as

$$\hat{p}_\phi \Psi(x, \phi) = \frac{\hbar}{i} \frac{d}{d\phi} \Psi(x, \phi), \quad (80)$$

$$\hat{x}_{\phi_0} \Psi(x, \phi) = \int_{-\infty}^{\infty} dk \left(\frac{1}{i} \frac{d}{dk} + \frac{k}{\beta_0 |k|} \phi_0 \right) f_>(k) e^{i \frac{|k|}{\beta_0} \phi} e^{-ik \ln l}, \quad l > 0, \quad (81)$$

$$= \int_{-\infty}^{\infty} dk \left(\frac{1}{i} \frac{d}{dk} + \frac{k}{\beta_0 |k|} \phi_0 \right) f_<(k) e^{i \frac{|k|}{\beta_0} \phi} e^{ik \ln |l|}, \quad l < 0, \quad (82)$$

where in (81),(82), $f_>(k), f_<(k)$ satisfy the appropriate conditions implied by replacing $f_\pm(\omega)$ by $f_{>\pm}(\omega), f_{<\pm}(\omega)$ on equation(57). Thus \hat{x}_{ϕ_0} is defined on a dense domain wherein $f_>(k), f_<(k)$ and all their derivatives vanish at $k = 0$ and $|k| \rightarrow \infty$.

The resultant representation on $L^2(R, |l|^{-1}dl)$ is exactly the Wheeler DeWitt representation of [3]. As in that work, the operator $\hat{\Pi}$ defined by $\hat{\Pi}|l\rangle = | - l \rangle$ is a large gauge transformation . This implies that physical positive frequency states lie in the symmetric sector of \mathcal{H}_{+phys}^* whose image under U is the symmetric sector of $L^2(R, |l|^{-1}dl)$ characterised by

$$F(k) := f_>(k) = f_<(-k). \quad (83)$$

This completes our analysis of the case wherein we drop (iii) of section 1.

Before we proceed to the next section wherein (iii) is retained we would like to stress an important technical issue overlooked by APS in their analysis of WDW states. It is very important that the domain of the operator \hat{x}_{ϕ_0} be defined carefully as we have done above. The wave functions in this domain are in Schwartz space i.e they fall off faster than any power of $\ln |l|$.

APS require that wave functions have Schwartz space behaviour in $\ln |l|$ (actually they require such behaviour in l which is difficult to implement) and they equate this requirement with Schwartz space behaviour of $F(k)$ in equation (83). However this is incorrect due to the presence of the $e^{i \frac{|k|}{\beta_0} \phi}$ term in the mode expansions. This term is not differentiable with respect to k at $k = 0$ and if $F(k)$ does not satisfy our requirements at $k = 0$, the resulting wave function has a power law fall off at infinity [9]. Further, APS choose $\hat{\mu}_{\phi_0}$ as their Dirac observable. Since this is exponentially related to \hat{x}_{ϕ_0} , this operator does not have well defined action on wave functions for

which $F(k)$ is merely Schwartz. This has important implications for their semiclassical analysis. APS choose $F(k)$ to be a Gaussian - hence it is not in our domain. In their evaluation of expectation values and fluctuations of $|\hat{\mu}|_{\phi_0}$ they neglect certain terms which, due to bad infrared behaviour in $\ln |l|$ contribute divergently [9]. As we shall show in a subsequent paper [9], the expectation value and fluctuations of \hat{x}_{ϕ_0} do exist in this state and behave reasonably. However, these technicalities are not expected to find their way into their LQC ‘quantum bounce’ results. The reason is that, amongst other checks, APS have evaluated the wave function in l, ϕ space by evaluating the relevant integral (see equations (77),(78),(83)) in k -space numerically and in their numerical evaluation they have used a function which is Gaussian near its peak but which is of compact support in k and whose support is outside $k = 0$.

6 The physical state space in the presence of Thiemann-like inverse triad definitions.

Let $B(\mu)$ be obtained from a Thiemann like prescription [5, 1] and set $l_0 = L = 0$. Since $\frac{dx}{dt} = B^{1/2}(\mu(l))$ and B obtained in [1, 2] or [3] is positive and non-vanishing except at $l = 0 = x(l = 0)$, it follows that x is an invertible function of l . Hence all the considerations of section 4 apply. In particular, the positive frequency eigen functions are doubly degenerate unlike in the WDW case. Symmetric states in \mathcal{H}_{+phys}^* or, equivalently, in $L^2(R, dx)$ are defined by $f_+(\frac{|k|}{\beta_0}) = f_-(\frac{|k|}{\beta_0})$ or, equivalently, $f(k) = f(-k)$ (see equation (67)).

From equations (54) and (55) it follows that

$$\frac{d\hat{x}_{\phi_0}}{d\phi_0} = \pm\beta_0^{-1}. \quad (84)$$

Thus implies that the corresponding classical evolution equations with respect to the scalar field ‘time’ are

$$\frac{dx(\phi)}{d\phi} = \pm\beta_0^{-1} \quad (85)$$

which have the solutions

$$x - x_* = \pm\beta_0^{-1}(\phi - \phi_*) \quad (86)$$

The expanding branch follows $x - x_* = \beta_0^{-1}(\phi - \phi_*)$ so that evolving backwards from some large x_* , the value $x = 0 = \mu$ is reached in finite scalar field-time. Thus the epoch when the size of the universe vanishes is reached in finite time. However,

- (a) the scalar field energy density, $\rho = (\frac{8\pi\gamma l_P^2}{6})^3 (p_\phi B(\mu))^2$ is bounded throughout and vanishes at $\mu = 0$.
- (b) there is regular evolution beyond the point at which the size of the universe vanishes.

In this sense the singularity is resolved. In the next section we discuss the freedom in defining B and argue that a choice of $B(\mu)$ exists for which the phenomenon of singularity resolution is independent of the choice of the fiducial cell \mathcal{V} which underlies the quantization (see section 2).

7 Is singularity resolution without curvature corrections physically well defined?

If we use the available choices of $B(\mu)$ in the literature [1, 2, 3], the following unphysical situation (pointed out by APS in [3]) is encountered. Typically $B(\mu)$ departs significantly from the WDW choice $|\mu|^{-3/2}$ when μ is close to some fixed μ_0 [1, 2] or when $v = \text{sgn}(\mu)\mu^{3/2}$ is close to 1 [3]. This is the stage at which quantum effects become important. However, $(\frac{8\pi\gamma l_P^2}{6})^{3/2}|v|$ is the volume of the fiducial cell \mathcal{V} with fiducial volume V_0 . Since the choice of \mathcal{V} is arbitrary, physical phenomena, such as the stage at which quantum effects become important, should not depend on this choice and therefore singularity resolution in the context of such a choice of B cannot be taken seriously.

The choice of B in the APS work [2, 3] is motivated by requiring that the physical length scale, associated with the loop which labels the holonomy which regulates the definition of $|\hat{p}|^{-3/2}$, be of order of the Planck length. This motivation, the consequent choices of holonomy operator in [2, 3] and the arguments mentioned above against the physical significance of singularity resolution due to inverse triad definitions, form one consistent viewpoint. Below we propose a different viewpoint, also self consistent, which motivates an alternate choice of B .

The LQC quantization requires a choice of fiducial metric and fiducial cell. These are auxilliary structures which facilitate the explicit imposition of homogeneity and isotropy and which allow the definition of spatial integrals, vital to the Hamiltonian framework, which would diverge if evaluated over non-compact spatial manifold. Their auxilliary nature requires, as mentioned above, that physical results do not depend on the particular choice. Let us first fix the fiducial metric (we shall relax this later). Then the only choice in the quantization is that of the fiducial cell. Denote two such choices by $\mathcal{V}_1, \mathcal{V}_2$ with fiducial volumes $V_{0,1}, V_{0,2}$. Fix the state $|v_1\rangle_1$ (v is related to μ as described above; $(\frac{8\pi\gamma l_P^2}{6})^{3/2}v$ is the eigen value of the volume operator, $|\hat{p}|^{3/2}$) in the first case. Then the physical volume of the

cell \mathcal{V}_1 is $(\frac{8\pi\gamma l_P^2}{6})^{3/2}v_1$. Similarly the physical volume of the cell \mathcal{V}_2 in the state $|v_2\rangle_2$ is $(\frac{8\pi\gamma l_P^2}{6})^{3/2}v_2$. Hence the physical volume of \mathcal{V}_1 in the state $|v_2\rangle_2$ is $\frac{v_2}{V_{0,2}}V_{0,1}$. Hence the states $|v_1\rangle_1$, $|v_1\frac{V_{0,2}}{V_{0,1}}\rangle_2$ describe the same physical spatial geometry. Hence the inverse volume of \mathcal{V}_1 in these states should also be identical. Denoting the inverse volume functions (modulo the factor $(\frac{8\pi\gamma l_P^2}{6})^{3/2}$) in the 2 cases by $B_1(v)$, $B_2(v)$, the above discussion implies that

$$B_1(v_1) = \frac{V_{0,2}}{V_{0,1}}B_2(\frac{V_{0,2}}{V_{0,1}}v_1). \quad (87)$$

This is not satisfied by the choices of B in [1, 2, 3]. It is, however, straightforward to check that if we replace the APS [3] holonomy operators $e^{\frac{i\bar{\mu}c}{2}}$ (see [3] for a definition of $\bar{\mu}$ and of this operator) by $e^{\frac{i\lambda_1\bar{\mu}c}{2}}$ in case 1 and $e^{\frac{i\lambda_2\bar{\mu}c}{2}}$ in case 2 then we have that for $i = 1, 2$

$$B_i(v) = (\frac{3}{2})^3 K |v| \{ \frac{|v + \lambda_i|^{1/3} - |v - \lambda_i|^{1/3}}{\lambda_i} \}^3, \quad (88)$$

where K is a numerical factor defined in [3]. If we set

$$\frac{\lambda_1}{\lambda_2} = \frac{V_{0,1}}{V_{0,2}} \quad (89)$$

then it follows straightforwardly that equation (87) holds. The choices (88), (89) not only yield the correct scaling (87) but mesh well with an alternate viewpoint on the significance of the holonomy operator, pointed out in [10]. The authors of that work note that the inverse triad is obtained classically by a derivative of the volume function V . In the LQG regularization this is replaced by a “discrete derivative” [10] through the structure $\hat{V} - \hat{h}^{-1}\hat{V}\hat{h}$ where \hat{h} is the holonomy operator. Indeed, in LQC, the APS holonomy operator [3] provides *exactly* such a realization of the regularization process by virtue of its being a displacement operator for $|v\rangle$. Viewed in this light, consider, once again the APS choice [3] for \hat{h} . For the quantization based on the fiducial cell \mathcal{V}_1 this operator increments the physical volume of \mathcal{V}_1 by the fixed amount $(\frac{8\pi\gamma l_P^2}{6})^{3/2}$. For the quantization based on \mathcal{V}_2 , the operator increments the physical volume of \mathcal{V}_2 by this same amount and consequently increments the physical volume of the cell \mathcal{V}_1 by the amount $(\frac{8\pi\gamma l_P^2}{6})^{3/2}\frac{V_{0,1}}{V_{0,2}}$. If we demand that the volume displacement be independent of the choice fiducial cell \mathcal{V} we again arrive at the modified operators $e^{\frac{i\lambda_1\bar{\mu}c}{2}}$, $e^{\frac{i\lambda_2\bar{\mu}c}{2}}$ with λ_1, λ_2 satisfying equation (89).

This implies that there is some region R of fiducial size $V_0(R)$ for which the physical volume increment is exactly $(\frac{8\pi\gamma l_P^2}{6})^{3/2}$ *independent* of the choice of \mathcal{V} so that $\lambda_i = \frac{V_{0,i}}{V_0(R)}$, $i = 1, 2$. At first sight this seems unphysical.

Note however that the spatial diffeomorphism gauge freedom is fixed so that the fiducial coordinates are of physical, gauge invariant relevance even though they are not metrical distances. The above discussion is predicated on a fixed choice of fiducial metric consistent with homogeneity and isotropy. However, as we describe below, our considerations are independent of this choice.

Our picture is as follows. Underlying the effective description provided by LQC, is a physical state of the full theory. The full theory has gravity, scalar field matter as well as suitable matter degrees of freedom which define physical spatial coordinates in a manner envisaged by, for example, Rovelli in [11]. Thus the underlying LQG state has enough structure to enable the definition of a class of physical coordinate systems on the spatial manifold Σ such that homogeneity and isotropy are manifest. Isotropy and homogeneity imply that these physical coordinate systems are related to each other by constant rescaling. These are just the set of all comoving coordinate systems.

Homogeneity itself is expected to arise as a good effective property after averaging out microphysics. The scale at which homogeneous modes are a sufficiently good description is time dependent- for example, a very large scale today is much smaller at an earlier epoch if the two epochs are part of an expanding phase. A time independent notion of the minimal domain wherein a homogeneous description is adequate can be stated in terms of comoving coordinates provided by the underlying LQG state as follows. Around any point $p \in \Sigma$, the LQG state defines a minimal region R_p wherein homogeneity is a good effective description. Homogeneity requires that R_p takes the form of a p independent comoving cell around p . This is exactly the cell R alluded to above.

The choice of comoving coordinates naturally defines a flat fiducial metric. Different choices endow the cell R with different fiducial sizes. Note that while the fiducial volume of R depends on the choice of comoving coordinates, R itself is independent of this choice.

As indicated above, LQC requires a choice of cell (in general different from R) as well as a fiducial metric. As we shall see explicitly below, introducing the λ dependent holonomies (see the discussion before (88)) ensures that inverse volume effects become important when the *physical* volume of the cell R approaches $(\frac{8\pi\gamma l_P^2}{6})^{3/2}$. This statement is independent of the LQC choice of cell and fiducial metric. We have already shown that the statement holds for a fixed fiducial metric. We now show that it also holds when we vary the choice of (comoving coordinates and associated) fiducial metric.

We define the following notation. For the LQC quantization choice of cell \mathcal{V}_k and comoving coordinate system $\{x\}_\alpha$, denote the fiducial volume of the cell by $V_{\alpha,k}$ and the volume eigenstates by $|v\rangle_{\alpha,k}$ so that $(\frac{8\pi\gamma l_P^2}{6})^{3/2}v$ is the physical volume of \mathcal{V}_k . Arguments identical to those for the case of fixed choice of fiducial metric, indicate that, in obvious notation, we must

identify the state $|v_{\alpha,k}\rangle_{\alpha,k}$ with the state $|v_{\beta,l}\rangle_{\beta,l}$ iff the eigenvalues $v_{\alpha,k}, v_{\beta,l}$ satisfy the relation

$$\frac{v_{\beta,l}}{v_{\alpha,k}} = \frac{V_{\beta,l}}{V_{\beta,k}} = \frac{V_{\alpha,l}}{V_{\alpha,k}}, \quad (90)$$

where we have used the fact that the α and β fiducial metrics are related by constant rescaling. The above equation shows that the identification of states is independent of the fiducial metric label α so that we may drop the α, β labels from the eigen values $v_{\alpha,k}, v_{\beta,l}$ and denote the identified pair of states by $|v_k\rangle_{\alpha,k}, |v_l\rangle_{\beta,l}$ with

$$\frac{v_l}{v_k} = \frac{V_{\gamma,l}}{V_{\gamma,k}} \forall \gamma, \quad (91)$$

where, once again, we have used the fact that all fiducial metrics are related by constant rescalings.

Next, denote the holonomy operators appropriate to the two sets of choices by $e^{\frac{i\lambda_{\alpha,k}\bar{\mu}c}{2}}, e^{\frac{i\lambda_{\beta,l}\bar{\mu}c}{2}}$. The action of the operators $e^{\frac{i\lambda_{\alpha,k}\bar{\mu}c}{2}}, e^{\frac{i\lambda_{\beta,l}\bar{\mu}c}{2}}$ on the states $|v_k\rangle_{\alpha,k}, |v_l\rangle_{\beta,l}$, yield the states $|v_k + \lambda_{\alpha,k}\rangle_{\alpha,k}, |v_l + \lambda_{\beta,l}\rangle_{\beta,l}$. In analogy to our arguments for the fixed fiducial metric case, we require that these operators increment the *physical* volume of R by the fixed amount $(\frac{8\pi\gamma l_P^2}{6})^{3/2}$. It is easy to check that this implies that

$$\lambda_{\alpha,k} = \frac{v_k}{v_R}, \quad \lambda_{\beta,l} = \frac{v_l}{v_R} \quad (92)$$

where $(\frac{8\pi\gamma l_P^2}{6})^{3/2}v_R$ denotes the physical volume of the region R in the state $|v_k + \lambda_{\alpha,k}\rangle_{\alpha,k}$. This volume is identical to that in the state $|v_l + \lambda_{\beta,l}\rangle_{\beta,l}$ by virtue of equation (91). Thus the λ factors are independent of the fiducial metric. This implies that the inverse volume functions (in obvious notation) $B_{\alpha,k}, B_{\beta,l}$ are independent of the fiducial metric labels α, β . This completes the argument.

8 Discussion

The simplicity of the Hamiltonian constraint for spatially flat, homogeneous and isotropic gravity coupled to a massless scalar field allows us to define its exponentiated square roots as unitary operators on the standard LQC kinematic Hilbert space [6] using a technique introduced in Reference [3]. This allows the application of group averaging methods coupled with some key ideas (see section 4) to construct the physical Hilbert space of the model without any of the higher order curvature corrections which occur in all previous LQC treatments of the model. This allows us to evaluate the role of various exotic features of LQC in the phenomenon of singularity resolution in the model.

As expected, from prior work [7, 12], our work confirms that the quantum bounce of the APS quantizations [2, 3] is clearly due to the higher order curvature corrections (see (ii) of the Introduction) to general relativistic dynamics which are present in their work. In the absence of such corrections we have demonstrated in sections 5 and 6 that the bounce does not occur. Remarkably, without such corrections, the kinematic discreteness of the LQC representation does not leave any imprint on our physical Hilbert space representations. Thus the physical Hilbert space representations of sections 5 and 6 do not split into an uncountable number of separable superselection sectors each characterised by a 1 dimensional regular lattice coordinatised by discrete values of the μ [2] or v [3] variables. Instead, the physical Hilbert space obtained in this work, by group averaging, is always separable and the variable x of section 6 ranges over the entire real line.⁵

If in addition to a curvature correction free LQC quantization of the model, one uses the straightforward spectral analysis based inverse scale factor operator to define the matter density, the physical Hilbert space representation turns out to be the WheelerDeWitt one. If one uses Thiemann-like [5, 6, 2, 3] definitions for the inverse scale factor operator the physical state representation is inequivalent to the WDW one and exhibits singularity resolution through well defined, regular (backward) evolution through the classically singular region. Such singularity resolution is physically unambiguous only if we slightly alter the definition of the APS “improved” inverse volume operator of Reference [3] along the lines indicated in section 7. Remarkably, the scaling requirements of section 7 *cannot* be satisfied for the triad independent holonomy operator of Reference [2]. Also remarkable, is that the scaling requirements *are* satisfied for all choices of Bojowald’s ambiguity parameter l (at least for the $j = 1/2$ case) [6] provided that his expressions are suitably generalised to the context of the triad dependent operators introduced in section 7.

As mentioned above, our considerations are tied to the simplicity of the Hamiltonian constraint of the model. While it is conceivable that our considerations may generalise to the spatially closed isotropic model (with a massless scalar field as in this work), we do not see how to apply our ideas to more complicated settings in which anisotropies play a role such as in the homogeneous diagonal models of Reference [13]. Thus, in the context of more general settings our results here can, at best, be viewed as suggestive of the nature of quantum inverse triad effects near singularities.

In our work, singularity resolution only depends on quantum effects which become important when the physical size of the region R (see section 7) becomes of the order of the Planck volume (assuming that the Immirzi

⁵Appendix C of Reference [2] details an $L^2(R)$ physical Hilbert space representation; however the representation still has traces of the kinematic discreteness characteristic of LQC by virtue of the role of a *difference* operator in the definition of quantum dynamics and Dirac observables.

parameter is of order unity). The mechanism of singularity resolution is thus independent of the matter density. Thus, the universe at large size could have an arbitrarily large matter density (by choosing p_ϕ to be arbitrarily large) and still behave classically. This is in contrast to the APS mechanism of singularity resolution in Reference [3] wherein the density is always bounded by the critical density at the bounce if the state at large volume is to be semiclassical. It would be of interest to compare our viewpoint (see section 7) on the physical validity of inverse volume operator driven singularity resolution with the “lattice refinement” picture of Bojowald [14], particularly the relation between the region R here and the lattice parameter l_0 in Reference [14].

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